2-Furancarboxamide, N-ethyl-

Inchi:	InChI=1S/C7H9NO2/c1-2-8-7(9)6-4-3-5-10-6/h3-5H,2H2,1H3,(H,8,9)
InchiKey:	VYCBCTICMMPTLJ-UHFFFAOYSA-N
Formula:	C7H9NO2
SMILES:	CCNC(=O)c1ccco1
Mol. weight [g/mol]:	139.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.97		Crippen Method
logp	1.029		Crippen Method
mcvol	107.450	ml/mol	McGowan Method
rinpol	1273.00		NIST Webbook
rinpol	1273.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407238&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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